Noise and Dynamical Pattern Selection in Solidification

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The overall goal of this project was to understand in more detail how a pattern-forming system can adjust its spacing. "Pattern-forming systems," in this context, are nonequilibrium contina whose state is determined by some experimentally adjustable control parameter. Below some critical value of the control parameter, the system remains in a simple steady state. Above critical, this state becomes unstable, and the system then has available to it a range of linearly stable, spatially periodic steady states, each characterized by a spacing which can lie anywhere within some band of values. These systems include interfacial systems like directional solidification, where the solidification front is planar when the ratio of growth velocity to thermal gradient is below its critical value, but takes on a cellular shape above critical. They also include systems without interfaces, such as Bénard convection, where it is the fluid velocity field which changes from zero to something spatially periodic as the control parameter is increased through its critical value.

The basic question to be addressed was that of how the system chooses one of its myriad possible spacings when the control parameter is above critical, and in particular the role of noise in this selection process. Previous work on explosive crystallization had suggested that one spacing in the range should be preferred, in the sense that weak noise should eventually drive the system to that spacing. That work had also suggested a heuristic argument for identifying the preferred spacing. The project had three main objectives: to understand in more detail how a pattern-forming system can adjust its spacing; to investigate how noise drives a system to its preferred spacing; and to extend the heuristic argument for a preferred spacing in explosive crystallization to other pattern-forming systems.

The project began with the first of these objectives. With an undergraduate student, Jed Overmann, I examined the process of pattern adjustment in the Swift-Hohenberg equation, which is a standard model of interfacial pattern formation, and some of its generalizations. These equations have linearly stable steady states of the form $A\sin(kx)$ for a range of wave number k. We developed numerical algorithms to find the "saddle" states, the ones which are intermediate between the steady state having N waves on a certain interval and the one having $N+1$ waves. After some exploration, we came to realize that these saddle states are essentially *phase perturbations* of the steady states, in which two of the N waves are pulled farther apart than the average spacing, with several neighboring waves pushed very slightly closer together. Depending on the detailed shape of the interface in the gap between the separated waves, a new wave may or may not form there, resulting in a return to the N-wave state or an adjustment to the $N+1$-wave state respectively. The relevance of this work to the overall project will be discussed below.

To address the second objective, I investigated the Fokker-Planck equation, which governs the probability distribution for states of a system subjected to noise. Let the front shape be given by its Fourier spectrum, with the component of wave number k having amplitude A_k. The evolution of the front shape is specified by equations for the time evolution of the A_k,

$$\dot{A}_k = F_k[\vec{A}]. \tag{1}$$

The notation $\vec{A}$ is a shorthand for the collection of all the A_k, and the dot represents a time derivative. The possible steady state front shapes are those for which all F_k vanish. For each k, we now add an independent Gaussian noise source with mean zero and variance η^2. This is the appropriate type of noise to add in order to test which steady state of (1) is preferred by the dynamics, since by giving each wave number equal power, the noise itself does not favor any wave number. The front shape $\vec{A}$ then becomes a random variable, and we seek its probability distribution $\mathcal{P}[\vec{A}]$. After an initial transient, this is given by the stationary Fokker-Planck equation,

$$0 = \frac{\partial}{\partial A_k}\left(F_k\mathcal{P} - \frac{\eta}{2}\frac{\partial \mathcal{P}}{\partial A_k}\right), \tag{2}$$

with summation over repeated indices implied. Note that the noise strength η multiplyies the highest derivative in the equation, so that the weak-noise limit, $\eta \to 0$, is singular. To solve (2) in this limit, we write the $\mathcal{P}$ in a WKB form,

$$\mathcal{P}[\vec{A}] = K[\vec{A}]\exp(-W[\vec{A}]/\eta)\,(1+O(\eta)). \tag{3}$$

Substituting this into (2) and expanding in powers of η yields equations for W and K. From (3) we see that the most probable state of the system in the weak-noise limit is that for which W is a minimum. Thus the correct way to determine the preferred state of the system is to compute W for each steady state, then find the one for which it has the lowest value.

An important special case arises when the deterministic equations (1) have a *gradient structure*, i.e., when we have $F_k[\vec{A}] = -\partial\Phi/\partial A_k$ for some scalar function $\Phi[\vec{A}]$. In this case, we have the exact solution

$\mathcal{P} = \exp(-2\Phi[\vec{A}]/\eta)$. Although most of the systems we are interested in do not have this structure, systems which do provide useful checks on the calculations. It is easy to see that the *deterministic* evolution (1) makes Φ decrease with time until the system reaches a steady state. Thus the linearly stable steady states are local minima of Φ. We found that W plays almost the same role for systems lacking a gradient structure: the deterministic evolution never increases W. In particular, linearly stable steady states of the deterministic dynamics are local minima of W.

These general considerations show that we need to calculate $W[\vec{A}]$ appearing in (3). The equation for W is

$$0 = \frac{\partial W}{\partial A_k}\left(\frac{1}{2}\frac{\partial W}{\partial A_k} + F_k\right). \tag{4}$$

This is the Hamilton-Jacobi equation at zero energy for the Hamiltonian $\mathcal{H}[\vec{p},\vec{A}] = |p|^2/2 + p_k A_k$, or the Lagrangian $\mathcal{L}[d\vec{A}/dt,\vec{A}] = (1/2)(\dot{A}_k - F_k)(\dot{A}_k - F_k)$, with W being the action,

$$W = \int \mathcal{L}\,dt = \int p_k\,dA_k. \tag{5}$$

To calculate the difference in W between two states, we should find the least-action path connecting those points and integrate along it according to (5). Least-action paths can be found by integrating the Lagrange equations in configuration space or the Hamilton equations in phase space. However, since $\mathcal{L}$ is manifestly positive, W must increase along the path. But a stable steady state is a local minimum of W, so least-action paths must all come *out* of such a state. Thus there cannot be a path from one stable steady state to another. To compare two steady states, we must integrate paths running from each steady state to some common point.

To clarify what is involved in these calculations, we have written numerical code for a simple case with only two degrees of freedom and two attractors. The deterministic equations are

$$\begin{aligned} \dot{x} &= x - x^3 - bxy^2, \\ \dot{y} &= \sigma y - cy^3 - dx^2 y. \end{aligned} \tag{6}$$

These equations have a gradient structure only for the special case $b = d$. They are obtained by taking a typical pattern-forming system in the weakly nonlinear regime (control parameter slightly above critical) and keeping only two Fourier modes, whose amplitudes are denoted here by x and y. All details of the particular model and the choice of which wave numbers to keep are embedded in the constants b, c, d, and σ. Note that these equations are not meant to be a serious model of any real pattern-forming system. Rather, we have studied them to clarify the issues that will arise when doing calculations for real systems, calculations which will need to be carried out in high-dimensional, rather than two dimensional, configuration spaces. The model in (6) has two attractors, one on the x axis and one on the y axis, whose basins are separated by a separatrix which contains a repeller at the origin and a saddle point. We found that there are paths satisfying the Lagrange equations which run from each attractor to the origin, but for $b \neq d$ one of these always crosses a caustic, and so is not a minimum of the action. Thus in order to compare the W values at the two attractors, we must find the least-action paths running from the attractors to the saddle, and so compare W at each attractor with W at the saddle. Note that a by-product of these calculations is the relative values of W between the attractors and the saddle. This turns out to give the exponential noise dependence of the rate of escape from each attractor, and so an estimate of the lifetimes of the linearly stable steady states.

The next step, which is currently under way, is to take what we have learned from our analytical calculations, our low-dimensional numerical calculations, and our search for saddle states, and devise practical numerical methods for comparing the W values of attractors in much higher dimensional systems. The attracting states are easy to calculate, since the time evolution of nearby states converges to them. We have developed methods of calculating the saddle states. What remains is to develop efficient methods for finding the least-action path from an attractor to its neighboring saddles. Two types of method are possible. Relaxation methods start with a trial path from the attractor to the saddle, then vary the path in order to minimize the action. With n points along the path in a d-dimensional space, this is a minimization over nd variables. The alternative is a shooting method, starting at the attractor, choosing an initial direction for the path, and integrating the Hamilton or Lagrange equations, then varying the initial direction in an attempt to hit the saddle. This is a minimization over only $d-1$ variables, but each trial takes much more

computation than moving a point along a trial path in the relaxation method. The relaxation method uses the fact that the solution path must go to the saddle, but not the fact that it must also satisfy the Lagrange equations, while the shooting method uses the latter fact but not the former. This is one of two directions this research has been taking since the conclusion of the contract.

Clearly the calculations which give the correct answer for the preferred spacing are difficult and involved. It would be much better if there were some vastly simpler way of finding the preferred spacing directly, without needing to calculate a variety of intermediate results. This is where the third objective comes in. A candidate for a simpler criterion arose in my earlier work on explosive crystallization; briefly, it is the conjecture that the preferred spacing is the one for which the growth rate of the Fourier amplitude, $\partial A_k/\partial t$, regarded as a function of k, has a maximum at the same wave number k for which A_k itself has a maximum. The third objective was to explore the relation between this criterion and the correct one, in an attempt to determine whether and under what circumstances the two give the same result, i.e., when the heuristic argument is correct.

We have been able to show that the heuristic criterion does indeed produce the correct preferred wave number when the deterministic equations have a gradient structure. The argument runs as follows. Suppose the free energy functional $\Phi[\vec{A}]$ is minimized among functions of the form $A_k = M\delta(k-q)$ with a *fixed* wave number q by $M = M_0(q)$. Denote the corresponding value of Φ by

$$\Phi_{min}(q) = \Phi[M_0(q)\delta(\cdot - q)]. \tag{7}$$

The preferred wave number will be the q value for which $\Phi_{min}(q)$ is a minimum. To find this, we calculate $\Phi_{min}(q+\delta q)$; at the preferred wave number, this will differ from $\Phi_{min}(q)$ by an amount which is of order $(\delta q)^2$. We find

$$\begin{aligned}
\Phi_{min}(q+\delta q) &= \Phi[M_0(q+\delta q)\delta(\cdot - q - \delta q)] \\
&= \Phi\left[M_0(q)\delta(\cdot - q) + \frac{dM_0}{dq}\delta(\cdot - q)\delta q - M_0(q)\delta'(\cdot - q)\delta q\right] \\
&= \Phi_{min}(q) + \delta q \int \frac{\delta\Phi}{\delta A_k}\left[\frac{dM_0}{dq}\delta(k-q) - M_0(q)\delta'(k-q)\right] dk \\
&= \Phi_{min}(q) + \frac{dM_0}{dq}\frac{\delta\Phi}{\delta A_k}\delta q + M_0(q)\frac{\partial}{\partial k}\left(\frac{\delta\Phi}{\delta A_k}\right)\delta q.
\end{aligned} \tag{8}$$

The functional derivative and its k-derivative appearing on the right side of the final equation are evaluated at $A_k = M_0(q)\delta(k-q)$ and $k = q$. Thus the second term on the right vanishes, since it is just the right side of the deterministic equations, $F_k[\vec{A}]$, evaluated at a fixed point. In order for q to be the minimum of Φ_{min}, the third term on the right must then vanish also; in other words, $\partial F_k/\partial k$, viewed as a function of k, must have a peak at $k = q$. This is precisely what the heuristic argument claims.

It is difficult to see how this argument can be generalized to systems which do not have a gradient structure. Indeed, general analytical results of any kind are difficult to come by in the non-gradient case. I am currently trying to work out the argument when the deterministic dynamics is close to a gradient system, that is when we have

$$F_k[\vec{A}] = -\frac{\partial\Phi}{\partial A_k} + \epsilon G_k[\vec{A}], \tag{9}$$

where ϵ is a small parameter. Adding the perturbation G_k generally shifts the positions of the fixed points of the dynamics, the deterministic trajectories, and the action-minimizing paths. Taking all this into account, we find that the difference in action between an attractor $\vec{A}^{(a)}$ and a saddle $\vec{A}^{(u)}$ is given, to first order in ϵ, by

$$W[\vec{A}^{(u)}] - W[\vec{A}^{(a)}] = 2\Phi[\vec{A}^{(u,0)}] - 2\Phi[\vec{A}^{(a,0)}] - 2\epsilon\int G_k[\vec{A}]\, dA_k, \tag{10}$$

where $\vec{A}^{(u,0)}$ and $\vec{A}^{(a,0)}$ are the unperturbed positions of the saddle and attractor, and the line integral is over the time-reversed, unperturbed deterministic trajectory which runs from the latter to the former. The next step, which is in progress, is to seek a relation between this result and the prediction of the heuristic criterion.